John von Neumann Institute for Computing

Oxydation of Methanol to Formaldehyde on V2O5 Investigated by Density Functional Theory

P. Boulet, F. Gilardoni, J. Weber, H. Chermette, A. Baiker, J.-C. Volta

published in

Modern Methods and Algorithms of Quantum Chemistry,
J. Grotendorst (Ed.), John von Neumann Institute for Computing, Jülich, NIC Series, Vol. **2**, ISBN 3-00-005746-3, p. 4, 2000.

http://www.fz-juelich.de/nic-series/

Oxydation Of Methanol to Formaldehyde On V_2O_5 Investigated By Density Functional Theory.

P. Boulet[1,2,4], F. Gilardoni[2], J.Weber[2], H. Chermette[1,2], A. Baiker[3] and J.-C. Volta[4]

[1] *Laboratoire de chimie physique théorique, Université Claude Bernard Lyon 1, Bât 210, 43 Bld du 11 novembre 1918, 69622 Villeurbanne cedex.*
[2] *Département de Chimie-Physique, Université de Genève, 30 Quai E-Ansermet, CH-1211 Genève 4.*
[3] *Laboratory of Technical Chemistry, ETH Zentrum CNB, CH-8092 Zürich, Switzerland.*
[4] *Institut de Recherches sur la Catalyse, CNRS, 2 av. Albert Einstein, 69626 Villeurbanne cedex.*

As a precursor to materials of industrial interest formaldehyde is one of the most widely used chemicals. One way to obtain formaldehyde is to dehydrogenate methanol on vanadium oxide-based catalysts. Lots of work remain to be accomplish to understand the chemical processes of the reaction.
In this poster, we present the adsorption of methanol and propose a mecanism for the mild oxidation.